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Determination of the optimal parameters of the structure of functional gradient materials using mathematical modelling approaches

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ABSTRACT

Purpose: Functioning of mechanical friction systems largely depends on the characteristics of the structure of their surface layers. By controlling these parameters, it is possible to significantly adjust the reliability and durability of parts under the conditions of contact interaction.

Design/methodology/approach: he proposed approach, which is based on the principle of nonlocality of the operational properties of materials, allows determining the optimal microhardness values of the surface layers and the gradient of this parameter, at which the contact durability of friction pair elements significantly increases.

Findings: It is established that by adjusting the ratios of the surface strength of materials and its gradient, it is possible to achieve a significant increase in the operational parameters of friction units.

Practical implications: The engineering relationship considered in the work allows to establish functional distributions of microhardness in the structure of surface layers, at which their wear reaches minimum values.

Originality/value: Mathematical approaches are proposed, which allow determining the parameters of the structure of the surface layers of parts to increase their durability under conditions of friction contact loads.

Keywords: Functional gradient materials, Microhardness, Wear, Optimal structure of tribosystem's material

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ANALYSIS AND MODELLING

1. Introduction

Determination of optimal coating parameters facilitating the increase of performance characteristics of critical structural elements in extreme working conditions is one of the key problems of modern tribology and surface engineering [1,2].

It does not seem possible to solve this problem based only on experimental research due to the difficulty of obtaining results and limited number of experimental data linking the structure of surface layers with the behaviour of tribosystems under contact interaction. This significantly limits the ability to make decisions, especially when applying multi-operational technologies for surface reinforcement of contact coupling components.

Using only analytical methods to solve this problem at present is impossible due to the complex type of distribution functions describing the structure and heterogeneous state of near-surface layers.

In this regard, it is promising to develop experimental-numerical methods for determining optimal distribution parameters of properties in near-surface layers, which on the back of limited prior information, allow establishing parameters of tribosystem components material structure capable to increase performance characteristics of frictional pairs.

2. Recent papers review

The fact that near-surface layers condition affects the behaviour of components under friction was established in the first papers in tribology at the beginning of the 20th century. Specifically, they associated the wear rate and the magnitude of applied load as well as hardness of a component material surface.

This type of dependencies is sufficiently convenient to be used in engineering practice and is therefore often found in reference literature [3,4].

In these types of dependencies, surface layer elasticity modulus, activation bonds energy, shear modulus, other physical, chemical parameters and geometrical characteristics of a surface layer may also be taken into account [5].

The development of mechanics and physical research methods resulted in a change in understanding of the nature of concepts "surface" and "surface layer" of a component. Previously, scientists interpreted surface as an interface. Now they view it as a boundary zone showing pronounced functionally graded properties depending on distinctive features of its formation [6].

This requires a significant modification of model representations since they allow taking into account features of the boundary zone structure and its influence on the performance behaviour of contact couplings.

Such researches are currently being conducted [7] though influence patterns of near-surface layers gradiency on the behaviour of components of frictional couplings in terms of contact interaction are underrepresented in the literature.

3. Statement of basic materials. General formulation of a problem

Optimal parametrisation of a component (product) coating structure is based on the following optimization problem.

Suppose at the reference time in the near-surface layer we have a functional distribution of properties $F(x,y,z)$. Following operation during time interval $[\tau_0;\tau_k]$ the wear rate, as one of coating parameters, equals $I[\tau_0;\tau_k]$. It's necessary to find such distribution $F^*(x,y,z)$, at which $I[\tau_0;\tau_k] \to \min$:

$$F^*(x,y,z):\ I[\tau_0;\tau_k] \to \min. \tag{1}$$

The problem presented in a symbolic form in expression (1) is solved according to the following scheme: let us assume that

$$I[\tau_0;\tau_k] = \int_{\tau_0}^{\tau_k} i(\tau)\,d\tau, \tag{2}$$

where $i(\tau)$ is a wear rate; let's present the wear rate as:

$$i(\tau)=\int_V i_Л(V,\tau)dV\,, \tag{3}$$

where $i_Л(V,\tau)$ is a local wear intensity, V is a body (product) volume at its initial configuration. Let us accept that

$$i_Л(V,\tau)\equiv G\big(F(x,y,z,\tau)\big), \tag{4}$$

where $G\big(F(x,y,z,\tau)\big)$ is a function that establishes connection between the structure and the wear rate in a local zone.

Since functional distribution of $F(x,y,z,\tau)$ properties is spatially heterogeneous, let us assume that in a local zone within the respective coordinate system it equals:

$$F(x,y,z,\tau)\approx F(x_0,y_0,z_0,\tau)+\frac{\partial F}{\partial x}x+\frac{\partial F}{\partial y}y+\frac{\partial F}{\partial z}z\,, \tag{5}$$

or

$$F(x,y,z,\tau)\approx F(x_0,y_0,z_0,\tau)+k_1x+k_2y+k_3z\,, \tag{6}$$

where $k_1=\frac{\partial F}{\partial x}$, $k_2=\frac{\partial F}{\partial y}$, $k_3=\frac{\partial F}{\partial z}$. To establish optimal parameters in local zones lets proceed to an integral estimation of structural characteristics according to the following equation:

$$F_{еф}=\frac{1}{\langle V\rangle}\int_{\langle V\rangle} F(x,y,z)\,dV\,, \tag{7}$$

where $\langle V\rangle$ is a regional value of integral averaging of local fields of property changes in the near-surface region. This region is dimensionally proportional to the dimensions corresponding to the features of contact loads under friction conditions – contact patches.

If we expand function $F(x,y,z,\tau)$ as in (6), an integral ratio (7) becomes:

$$F_{еф}=\frac{1}{L_1L_2L_3}\int_{L_1}\int_{L_2}\int_{L_3}F(x,y,z)dxdydz=$$

$$=\frac{1}{L_1L_2L_3}\int_{L_1}\int_{L_2}\int_{L_3}\big(F(x_0,y_0,z_0)+k_1x+k_2y+k_3z\big)dxdydz=$$

$$=F(x_0,y_0,z_0,\tau)+k_1\frac{L_1}{2}+k_2\frac{L_2}{2}+k_3\frac{L_3}{2}\,, \tag{8}$$

where L_i is a characteristic size of region $\langle V\rangle$ in *i*-th dimension.

Taking into account (8), relation (4) is as follows:

$$i_Л(V,\tau)\equiv G(F(x_0,y_0,z_0,\tau)+k_1(\tau)\frac{L_1}{2}+$$
$$+k_2(\tau)\frac{L_2}{2}+k_3(\tau)\frac{L_3}{2})\,. \tag{9}$$

Consequently, expression (9) takes into account the concept of "tribocontact near-surface zone" more fully be means of introduction of both values L_1, L_2, L_3 and graded properties of near-surface layers. If the above characteristics are neglected in relation (9), this expression turns into classical wear laws presented in tribology works, in particular in [4,8].

To solve problem (1) in general let's use the following scheme: let's assume that expression $I[\tau_0;\tau_k]\to\min$ is equivalent to relation $\sup\limits_{\tau\in[\tau_0;\tau_k]} i(\tau)\to\min$, which is identical to

$$G\left(F(x_0,y_0,z_0,\tau)+k_1(\tau)\frac{L_1}{2}+k_2(\tau)\frac{L_2}{2}+k_3(\tau)\frac{L_3}{2}\right)\to\min$$

at $\tau\in[\tau_0;\tau_k]$.

The task of mathematical modelling is to determine such $F(x_0,y_0,z_0,\tau)$, $k_1(\tau)$, $k_2(\tau)$, $k_3(\tau)$ so that for any time interval $\tau\in[\tau_0;\tau_k]$ wear rate $i(\tau)$ is minimal.

4. Solving of an applied problem for determining optimal parameters of tribosystem rolling surface structure

4.1. Empirical information

As the initial information used for predicting optimal structure of surface layers we use microhardness distribution obtained on 45 grade steel samples (HRC=38, R_a=0.57 μm), tested under unsteady rolling friction in a grease medium at various slip coefficient. Maximum Hertzian contact stress was 250 MPa. Table 1 shows the total wear values for these samples.

To determine optimal parameters of surface layers structure according to expression (9), it is *apriori* accepted that performance properties of samples (wear) depend both on surface layer microhardness characteristics and its distribution depthward a material:

$$I=G(HV(x))\,, \tag{10}$$

where HV is a microhardness value, x is a variable describing the depth up to which the sought characteristic changes from the surface of a component.

Therefore, as a measure of function G, an integral averaging of the distribution of microhardness is admitted:

$$G(HV(x)) = HV_{ef} = \frac{1}{L}\int_{L} HV(x)dx\,, \qquad (11)$$

where x is the value of a given depth characteristic in µm.

In a linear one-dimensional approximation function $HV(x)$ taken the form of:

$$HV(x) = HV_0 + k\cdot x\,, \qquad (12)$$

where x is microhardness at the surface, MPa, k is a value of microhardness gradient, MPa/µm.

Table 1.
Results of measurement of microhardness of samples and their performance characteristics

Samples	Microhardness value HV, MPa								Total wear of surfaces, µm
	Distance from a surface, µm								
	10	20	30	40	50	60	70	80	
Sample 1 (slippage 3%)	3451	3451	3451	3708	3708	3853	4010	4179	5.96
Sample 2 (slippage 10%)	3575	4564	5570	5570	5287	5023	5023	4783	3.83
Sample 3(slippage 20%)	3336	3451	3575	3853	5899	5570	5570	5570	4.27
Sample 4 (slippage 30%)	4023	5023	5287	5287	5570	6255	6255	7095	5.08
Sample 5 (slippage 40%)	4023	5287	5287	5287	5570	5570	6255	6255	6.11

A measure of strengthening of metallic near-surface layers for some depth depends on the rate of contact surfaces slippage. When a slipping rate increases from 0.062 to 1.15 m/s, which corresponds to the increase of slippage measure from 3 to 40% respectively, processes of heat liberation at tribological contact site become intensified and the gradient of lubricating layers displacement velocity increases, consequently the prerequisites for destruction of formed lubricant boundary films are created. Accordingly, the propagation area of shear stresses depthward the metal increases and stress-strain local zones in near-surface layers appear. Notwithstanding slipping rate, in the near-surface layers of surface material a rule of a positive gradient of mechanical properties per depth is materialised, which is an important mechanism in terms of increasing the wear resistance of frictional pairs.

Taking into account (12), relation (11) is as follows:

$$H_{ef} = F(H(x)) = \frac{1}{L}\left(H_0\cdot L + k\cdot\frac{L^2}{2}\right) = H_0 + k\cdot\frac{L}{2}. \qquad (13)$$

This parameter of effective microhardness is an average indicator of microhardness distribution in some local area encompassing the depth of distribution of elastic-plastic deformations at friction. This parameter is a strength criterion characterising spatial heterogeneity of microhardness distribution occurred as a result of operational modification of contact surfaces at friction.

Let us assume the value of microhardness at a depth 10 µm (Table 1, column 2) as the surface microhardness value and define a gradient as a ratio of difference between values of microhardness at a depth of 80 µm and 10 µm. This way we can obtain the dependence of wear on the effective microhardness, surface microhardness and gradient, which is presented in Table 2.

Table 2.
Dependence of material performance characteristics on generalized parameters of microhardness distribution

Samples	Surface microhardness, MPa	Gradient, MPa/µm	H_{ef}, MPa	Total wear of surfaces, µm
Sample 1 (slippage 3%)	3451	10.4	3857	5.96
Sample 2 (slippage 10%)	3575	17.2	4263	3.83
Sample 3 (slippage 20%)	3336	31.9	4612	4.27
Sample 4 (slippage 30%)	4023	43.8	5775	5.08
Sample 5 (slippage 40%)	4023	31.8	5295	6.11

4.2. Results of forecasting

Let us define interpolation analytical dependence of the amount of wear of surface I on the value of effective microhardness H based on results shown in Table 2:

$$I = 833.2181630 - 0.6016932517 * H + 0.1584466714 * 10^{(-3)} * H^2 - 1.778035727 * 10^{(-8)} * H^3 + 7.074211011 * 10^{(-13)} * H^4 , \quad (14)$$

where H is a value of effective ("integral") microhardness, $H \in [3800 \text{ MPa}; 5300 \text{ MPa}]$.

Let us plot characteristic curve *I(H)* (Fig. 1).

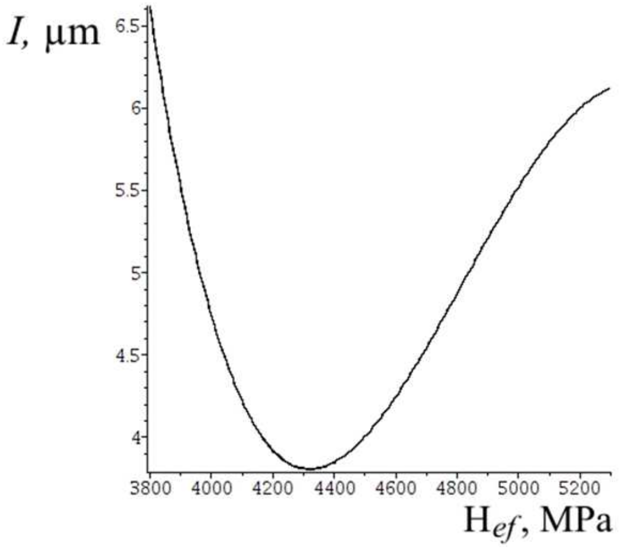

Fig. 1. Dependence of wear value I on parameter H_{ef}

As it can be seen from Figure 1, the above dependence reaches the minimum wear at microhardness value falling within the range from 4200 MPa to 4400 MPa.

Let us solve a problem of finding the value of effective microhardness, which provides a minimum value of wear I:

$$H^*_{ef} : I \to \min . \quad (15)$$

The task like (6) is equivalent to the following system of equations:

$$H^*_{ef} : \begin{cases} \dfrac{\partial I}{\partial H} = 0 \\ \dfrac{\partial^2 I}{\partial H^2} > 0 \end{cases} . \quad (16)$$

Let us find $H^*_{ef} = 4323 \ MPa$ from this system. A that, the predicted value of wear will be 3.80 μm.

It is necessary to note that achieving such value of effective microhardness, at which frictional pairs wear at a minimum level, is possible either by changing the surface microhardness value or by adjusting the value of its gradient. For instance, at set microhardness value of 3.575 MPa, the value of microhardness gradient must equal $k = \dfrac{2 \cdot (4323 - 3575)}{80} = 18.7$ MPa/μm. If gradient equals 17.2 MPa/μm, the surface microhardness value must be $H_0 = \left(4323 - \dfrac{1}{2} \cdot 17.2 \cdot 80 \right) = 3635$ MPa.

5. Conclusions

1. The problem of determining optimal parameters of properties of 3-D gradient materials of tribosystems within the amount of limited information on experimental tests was considered.
2. As a measure of functional distribution of surface layer local characteristics an integral averaging of microhardness value in a microvolume is admitted and then compared with the wear of a friction assembly.
3. The suggested approach allows determining optimal distribution of microhardness of surface layers of tribosystems for material justification and providing recommendations on the modes of technological and operational modification of friction assembly components in order to increase their wear resistance.

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